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Heterogeneity of Intercalated YBCO Single Crystals Determined by Polarized Cl *K*-, Br *K*-, and I- L_3 Edge XANES Analysis

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Beamline(s): X19A, X18B

Introduction: We have performed polarized Cl *K*-, Br *K*-, and I- L_3 edge XANES measurements on chlorinated, brominated, and iodinated underdoped single crystals of $YBa_2Cu_3O_{6+y}$ (y~0.3-0.5) showing a recovery of super-conductivity. This work is motivated to explore the effect of chlorination and iodination on electronic and the local structure of YBCO. In conjunction to our recently reported data on brominated sample [1], this would provide a systematic study of the intercalation phenomena. A key question is whether the halogen atom enters the lattice doping the system or if it cases a local decomposition reaction to occur, liberating oxygen, and re-oxygenating the underdoped unreacted regions. A general belief is that large iodine atoms cannot be accommodated, while small chlorine atoms occupy the O(1) vacancies (in Cu(1)-O(1) containing plains) doping the system.

Methods and Materials: Diffraction patterns of the intercalated samples revealed no evidence of the secondary phases. Cl *K*- and I L_3- edge polarized XANES spectra were collected at X19A in FY, using a 13-element Ge detectors with energy resolution of ~260 eV and a PIPS detector.

Results: Similar to the brominated sample [1] no visible polarization dependencies are observed at Cl *K*- and I L_3-edges. To ascertain this behavior MS simulations were performed on large clusters of atoms centered at Cl and I absorbers. Calculated Cl *K*-edge XANES (with Cl being placed into the O(1) position) showed marked polarization dependence, ruling out the doping scenario. Satisfactory results were obtained for *unpolarized* XANES, when either of halogen atoms substitutes Cu in the Cu(1) position in the reduced cluster of atoms (fragment of original YBCO lattice). Complementary EXAFS analysis supporting these finding for brominated and iodinated samples can be found elsewhere [1,2].

Conclusions: XANES results provide clear evidences that neither heavy Br and I nor light Cl atoms enter the perfect YBCO lattice. The intercalated samples becomes strongly heterogeneous on atomic length scales since the nano fragments about halogen atoms are found to be randomly oriented and incorporated into the well ordered "host" lattice of YBCO.

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References: [1] L. M. Dieng, A. Yu. Ignatov, T. A. Tyson, M. Croft, F. Dogan, C. -Y. Kim, J. C. Woicik and J. Grow, "Observation of Changes in the Atomic and Electronic Structure of Single-Crystal $YBa_2Cu_3O_{6.6}$ Accompanying Bromination", Phys. Rev. B **66**, (2002), *014501-014513*.
[2] A.Yu. Ignatov, L. M. Dieng, T. A. Tyson, M. Croft, W. Caliebe and S. Khalid. " Local Structure about I Atoms in Iodinated YBCO Single Crystals Determined by I- L_3 edge EXAFS Analysis ", NSLS'-02 Annual Report, Abstract No. Igna0561.